



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:03 AM UTC

PDB ID : 1WRA / pdb_00001wra
Title : Crystal Structure of Phosphorylcholine Esterase Domain of the Virulence Factor Choline Binding Protein E from Streptococcus Pneumoniae
Authors : Garau, G.; Dideberg, O.
Deposited on : 2004-10-13
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

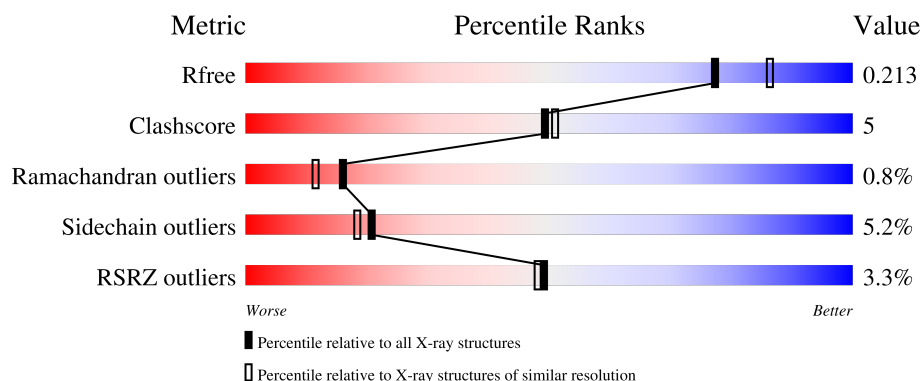
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

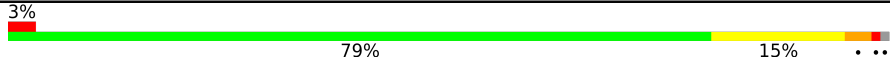
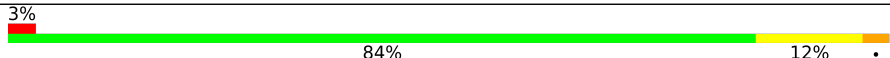
The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	308	
1	B	308	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5421 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Teichoic acid phosphorylcholine esterase/choline binding protein E (cbpE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	2	0
			2460	1546	421	490	3			
1	B	308	Total	C	N	O	S	0	1	0
			2480	1557	423	497	3			

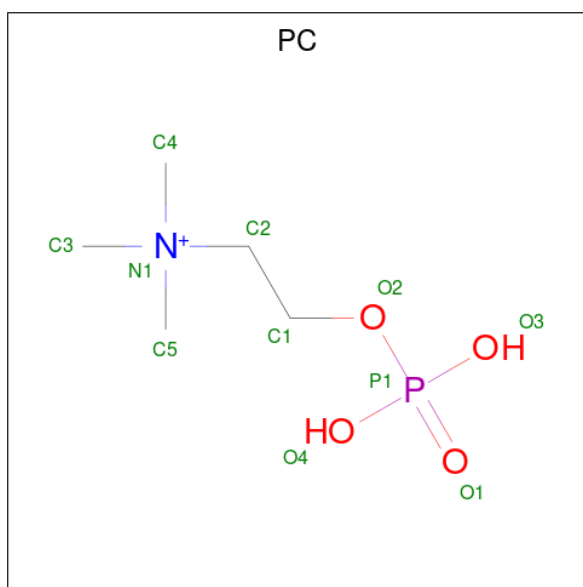
- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

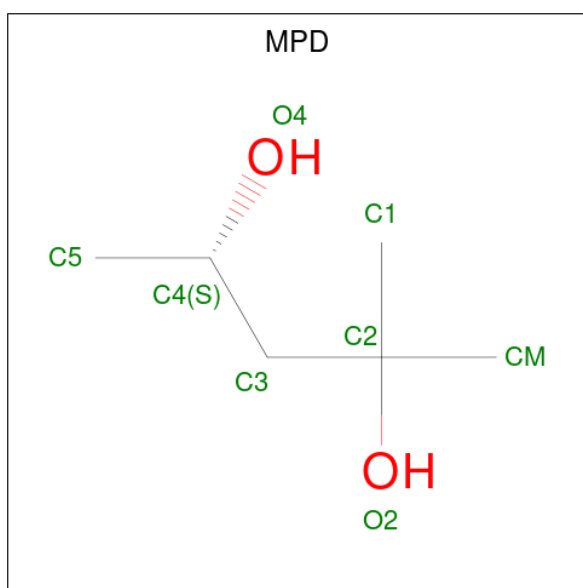
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PHOSPHOCHOLINE (CCD ID: PC) (formula: C₅H₁₅NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

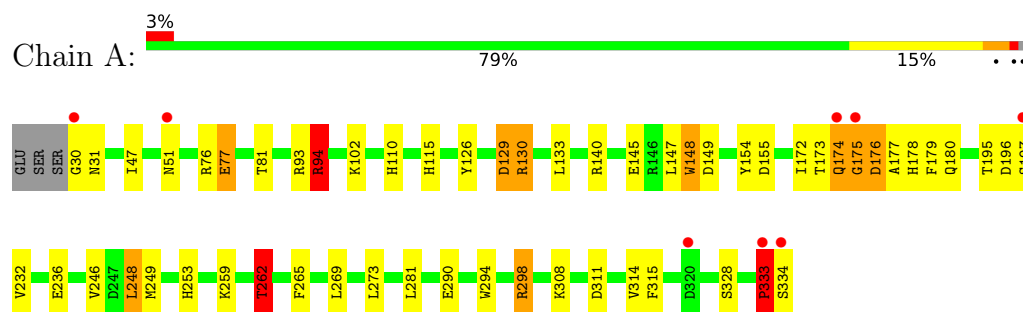
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	167	Total	O	0	1
			168	168		

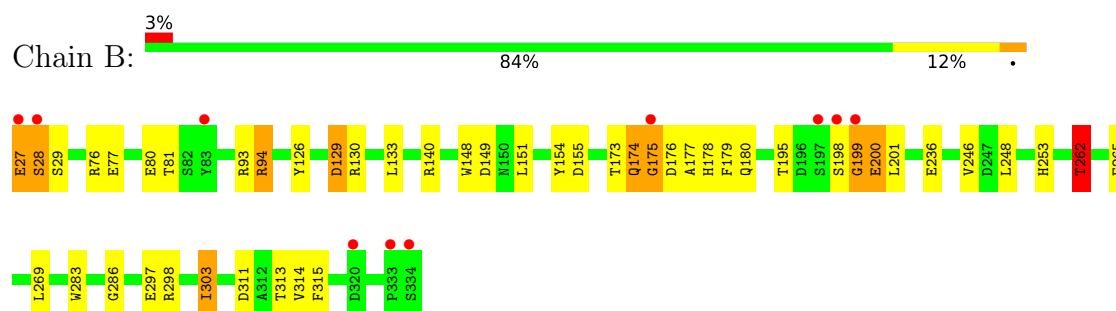
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Teichoic acid phosphorylcholine esterase/choline binding protein E (cbpE)



- Molecule 1: Teichoic acid phosphorylcholine esterase/choline binding protein E (cbpE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.30Å 98.30Å 172.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.84 – 2.00 23.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (23.84-2.00) 96.7 (23.84-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.38 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.174 , 0.204 0.188 , 0.213	Depositor DCC
R_{free} test set	2835 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5421	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC, FE, MPD, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	3/2527 (0.1%)	1.20	22/3419 (0.6%)
1	B	0.87	1/2539 (0.0%)	1.15	19/3436 (0.6%)
All	All	0.88	4/5066 (0.1%)	1.18	41/6855 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	10
All	All	0	22

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	ASP	CB-CG	-6.16	1.36	1.52
1	A	149	ASP	CA-CB	5.94	1.64	1.53
1	B	149	ASP	CB-CG	-5.78	1.37	1.52
1	A	262	THR	CA-C	5.19	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASP	N-CA-C	-13.40	95.34	112.90
1	B	155	ASP	N-CA-C	-12.02	95.75	112.45
1	B	77	GLU	N-CA-C	-11.12	91.29	109.96
1	A	77	GLU	N-CA-C	-9.73	93.61	109.96
1	A	315	PHE	N-CA-C	9.73	125.09	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	GLN	N-CA-C	9.39	123.84	112.38
1	A	180	GLN	N-CA-C	-9.21	93.20	108.76
1	B	180	GLN	N-CA-C	-9.16	93.27	108.76
1	B	315	PHE	N-CA-C	8.85	124.28	109.76
1	A	81	THR	N-CA-C	-8.46	104.09	114.75
1	A	174	GLN	N-CA-C	7.79	124.12	113.37
1	B	178	HIS	N-CA-C	7.68	121.44	109.07
1	A	148	TRP	CA-C-N	7.61	135.09	122.54
1	A	148	TRP	C-N-CA	7.61	135.09	122.54
1	A	178	HIS	N-CA-C	7.51	121.17	109.07
1	B	130	ARG	N-CA-C	7.38	118.34	108.38
1	A	149	ASP	CB-CG-OD1	-7.12	102.03	118.40
1	B	94	ARG	NE-CZ-NH2	-6.97	112.92	119.20
1	A	333	PRO	CA-C-O	-6.85	113.32	121.67
1	B	81	THR	N-CA-CB	6.65	121.72	110.49
1	B	262	THR	N-CA-CB	-6.49	99.38	109.69
1	B	149	ASP	CB-CG-OD1	-6.41	103.67	118.40
1	A	130	ARG	N-CA-C	6.32	116.91	108.38
1	B	149	ASP	CB-CG-OD2	6.32	132.94	118.40
1	A	178	HIS	N-CA-CB	-6.29	100.69	110.57
1	A	149	ASP	CB-CG-OD2	6.28	132.85	118.40
1	B	130	ARG	N-CA-CB	-6.19	101.46	111.24
1	B	148	TRP	CA-C-N	6.01	132.46	122.54
1	B	148	TRP	C-N-CA	6.01	132.46	122.54
1	A	262	THR	N-CA-CB	-5.98	99.70	109.56
1	B	178	HIS	N-CA-CB	-5.82	101.43	110.57
1	B	149	ASP	N-CA-CB	-5.77	101.95	110.49
1	A	262	THR	CB-CA-C	5.71	118.62	109.61
1	B	94	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	94	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	B	129	ASP	CB-CA-C	-5.60	98.41	109.67
1	A	130	ARG	N-CA-CB	-5.50	102.55	111.24
1	A	149	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	333	PRO	CA-C-N	5.39	131.40	121.70
1	A	333	PRO	C-N-CA	5.39	131.40	121.70
1	A	81	THR	N-CA-CB	5.21	118.76	111.15

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	129	ASP	Peptide
1	A	154	TYR	Peptide
1	A	175	GLY	Mainchain,Peptide
1	A	177	ALA	Peptide
1	A	179	PHE	Peptide
1	A	197	SER	Peptide
1	A	199	GLY	Peptide
1	A	314	VAL	Peptide
1	A	333	PRO	Peptide
1	A	76	ARG	Peptide
1	B	126	TYR	Peptide
1	B	129	ASP	Peptide
1	B	154	TYR	Peptide
1	B	175	GLY	Peptide
1	B	177	ALA	Peptide
1	B	179	PHE	Peptide
1	B	199	GLY	Peptide
1	B	314	VAL	Peptide
1	B	76	ARG	Peptide
1	B	80	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2460	0	2358	29	0
1	B	2480	0	2377	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	11	0	13	1	0
4	B	11	0	13	1	0
5	A	48	0	84	4	0
5	B	40	0	70	1	0
6	A	195	0	0	3	0
6	B	168	0	0	4	0
All	All	5421	0	4915	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HD2	1:A:311:ASP:OD2	1.72	0.89
1:B:27:GLU:HG3	1:B:28:SER:N	1.91	0.86
1:B:28:SER:N	1:B:29:SER:HA	2.00	0.75
1:A:236:GLU:OE1	1:A:262:THR:HB	1.87	0.75
1:B:195:THR:HB	1:B:199:GLY:HA3	1.70	0.73
1:A:173:THR:O	1:A:175:GLY:HA3	1.90	0.72
1:B:199:GLY:HA2	1:B:200:GLU:O	1.89	0.72
1:A:173:THR:C	1:A:175:GLY:HA3	2.20	0.67
1:B:236:GLU:OE1	1:B:262:THR:HB	1.97	0.64
1:A:30:GLY:HA3	1:A:51:ASN:H	1.65	0.60
1:B:195:THR:HB	1:B:199:GLY:CA	2.33	0.58
1:A:248:LEU:HD22	1:A:273:LEU:HD23	1.85	0.58
5:A:502:MPD:H12	5:A:502:MPD:H52	1.86	0.56
5:A:505:MPD:H52	5:A:505:MPD:HM1	1.89	0.55
1:A:195:THR:HB	1:A:199:GLY:CA	2.38	0.54
1:A:246:VAL:HG22	1:A:269:LEU:HB3	1.88	0.54
1:B:93:ARG:HD2	1:B:311:ASP:OD2	2.08	0.54
1:B:173:THR:C	1:B:175:GLY:HA3	2.34	0.53
1:B:262:THR:HG22	1:B:265:PHE:HB2	1.92	0.52
1:A:199:GLY:HA2	1:A:200:GLU:O	2.11	0.51
1:B:262:THR:HG21	6:B:1626:HOH:O	2.11	0.51
1:A:262:THR:HG22	1:A:265:PHE:HB2	1.93	0.50
1:A:195:THR:HB	1:A:199:GLY:HA3	1.93	0.50
1:B:262:THR:CG2	6:B:1626:HOH:O	2.59	0.50
1:A:196:ASP:OD1	1:A:199:GLY:N	2.44	0.50
1:A:253:HIS:HE2	4:A:501:PC:P1	2.34	0.49
5:B:1506:MPD:H53	5:B:1506:MPD:HM1	1.94	0.48
1:B:174:GLN:O	1:B:174:GLN:HG2	2.12	0.47
1:B:283:TRP:CZ2	1:B:286:GLY:HA2	2.49	0.47
1:A:294:TRP:CZ2	1:A:298[B]:ARG:HD3	2.50	0.47
1:A:333:PRO:HA	1:A:334:SER:CB	2.45	0.47
1:A:102:LYS:NZ	1:A:129:ASP:OD1	2.37	0.46
5:A:504:MPD:H12	5:A:504:MPD:H52	1.97	0.46
1:A:262:THR:HG21	6:A:650:HOH:O	2.16	0.46
1:A:94:ARG:HD3	6:A:690:HOH:O	2.15	0.46
1:A:262:THR:CG2	6:A:650:HOH:O	2.63	0.45
1:B:28:SER:H	1:B:29:SER:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:HD11	1:B:313:THR:HG21	1.98	0.45
5:A:503:MPD:H12	5:A:503:MPD:H52	1.99	0.45
1:A:172:ILE:HG23	1:A:176:ASP:HB3	1.98	0.44
1:A:30:GLY:HA2	1:A:31:ASN:HA	1.76	0.44
1:B:248:LEU:C	1:B:248:LEU:HD23	2.44	0.42
1:A:110:HIS:CE1	1:A:115:HIS:CD2	3.06	0.42
1:B:246:VAL:HG22	1:B:269:LEU:HB3	2.00	0.42
1:B:174:GLN:O	6:B:1601:HOH:O	2.21	0.42
1:A:259:LYS:HE2	6:B:1537:HOH:O	2.20	0.42
1:B:28:SER:HB2	1:B:29:SER:C	2.45	0.41
1:A:232:VAL:HG13	1:B:28:SER:HA	2.01	0.41
1:A:147:LEU:O	1:A:148:TRP:C	2.63	0.41
1:A:294:TRP:O	1:A:298[B]:ARG:HG3	2.21	0.41
1:A:195:THR:HB	1:A:199:GLY:HA2	2.04	0.40
1:A:294:TRP:CZ2	1:A:298[A]:ARG:HD3	2.56	0.40
1:A:249:MET:HG3	1:A:269:LEU:HD12	2.04	0.40
1:B:253:HIS:HE2	4:B:501:PC:P1	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/308 (99%)	289 (95%)	14 (5%)	2 (1%)	18	14
1	B	307/308 (100%)	292 (95%)	12 (4%)	3 (1%)	12	8
All	All	612/616 (99%)	581 (95%)	26 (4%)	5 (1%)	16	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ASP

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Mol	Chain	Res	Type
1	A	200	GLU
1	B	176	ASP
1	B	200	GLU
1	B	28	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/278 (100%)	258 (93%)	19 (7%)	14	11
1	B	279/278 (100%)	267 (96%)	12 (4%)	26	25
All	All	556/556 (100%)	525 (94%)	31 (6%)	21	16

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	77	GLU
1	A	94	ARG
1	A	130	ARG
1	A	133	LEU
1	A	140	ARG
1	A	145	GLU
1	A	174	GLN
1	A	198	SER
1	A	200	GLU
1	A	201	LEU
1	A	248	LEU
1	A	262	THR
1	A	281	LEU
1	A	290	GLU
1	A	298[A]	ARG
1	A	298[B]	ARG
1	A	308	LYS
1	A	328	SER

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Mol	Chain	Res	Type
1	B	27	GLU
1	B	94	ARG
1	B	133	LEU
1	B	140	ARG
1	B	151	LEU
1	B	198	SER
1	B	201	LEU
1	B	262	THR
1	B	297	GLU
1	B	298[A]	ARG
1	B	298[B]	ARG
1	B	303	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	285	ASN
1	B	187	GLN
1	B	210	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	B	1504	-	7,7,7	0.52	0	9,10,10	0.87	0
5	MPD	A	505	-	7,7,7	0.54	0	9,10,10	0.63	0
5	MPD	A	502	-	7,7,7	0.40	0	9,10,10	0.64	0
4	PC	A	501	2	10,10,10	1.49	1 (10%)	15,15,15	1.03	1 (6%)
5	MPD	B	1502	-	7,7,7	0.41	0	9,10,10	0.44	0
5	MPD	A	504	-	7,7,7	0.43	0	9,10,10	0.44	0
5	MPD	B	1503	-	7,7,7	0.42	0	9,10,10	0.39	0
5	MPD	A	507	5	7,7,7	0.47	0	9,10,10	0.49	0
5	MPD	B	1506	-	7,7,7	0.52	0	9,10,10	0.49	0
4	PC	B	501	2	10,10,10	1.09	1 (10%)	15,15,15	1.35	2 (13%)
5	MPD	A	506	5	7,7,7	0.45	0	9,10,10	0.26	0
5	MPD	B	1505	-	7,7,7	0.50	0	9,10,10	0.69	0
5	MPD	A	503	-	7,7,7	0.39	0	9,10,10	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	B	1504	-	-	2/5/5/5	-
5	MPD	A	505	-	-	1/5/5/5	-
5	MPD	A	502	-	-	4/5/5/5	-
4	PC	A	501	2	-	6/8/8/8	-
5	MPD	B	1502	-	-	5/5/5/5	-
5	MPD	A	504	-	-	2/5/5/5	-
5	MPD	B	1503	-	-	5/5/5/5	-
5	MPD	A	507	5	-	2/5/5/5	-
5	MPD	B	1506	-	-	1/5/5/5	-
4	PC	B	501	2	-	6/8/8/8	-
5	MPD	A	506	5	-	0/5/5/5	-
5	MPD	B	1505	-	-	2/5/5/5	-
5	MPD	A	503	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	PC	P1-O1	4.36	1.64	1.50
4	B	501	PC	P1-O4	2.65	1.64	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	PC	O4-P1-O3	3.72	121.73	107.80
4	B	501	PC	O2-P1-O1	2.21	112.41	106.44
4	A	501	PC	O4-P1-O1	2.11	119.05	110.83

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	PC	C1-O2-P1-O3
4	A	501	PC	C1-O2-P1-O4
4	B	501	PC	C1-O2-P1-O1
4	B	501	PC	C1-O2-P1-O3
4	B	501	PC	C1-O2-P1-O4
5	A	502	MPD	C2-C3-C4-O4
5	A	502	MPD	C2-C3-C4-C5
5	A	503	MPD	C2-C3-C4-O4
5	A	503	MPD	C2-C3-C4-C5
5	A	504	MPD	C2-C3-C4-O4
5	A	504	MPD	C2-C3-C4-C5
5	B	1502	MPD	C2-C3-C4-C5
5	B	1503	MPD	C2-C3-C4-O4
5	B	1503	MPD	C2-C3-C4-C5
5	B	1504	MPD	C2-C3-C4-C5
5	B	1505	MPD	C2-C3-C4-C5
5	B	1506	MPD	C2-C3-C4-C5
4	A	501	PC	C1-C2-N1-C3
4	B	501	PC	C1-C2-N1-C3
4	A	501	PC	C1-C2-N1-C4
4	B	501	PC	C1-C2-N1-C4
4	A	501	PC	C1-C2-N1-C5
4	B	501	PC	C1-C2-N1-C5
4	A	501	PC	C1-O2-P1-O1
5	B	1505	MPD	O2-C2-C3-C4
5	B	1502	MPD	C2-C3-C4-O4
5	A	505	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	B	1502	MPD	CM-C2-C3-C4
5	B	1503	MPD	CM-C2-C3-C4
5	A	502	MPD	O2-C2-C3-C4
5	B	1502	MPD	O2-C2-C3-C4
5	B	1503	MPD	O2-C2-C3-C4
5	B	1504	MPD	O2-C2-C3-C4
5	A	502	MPD	C1-C2-C3-C4
5	A	507	MPD	C1-C2-C3-C4
5	A	507	MPD	CM-C2-C3-C4
5	B	1502	MPD	C1-C2-C3-C4
5	B	1503	MPD	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	MPD	1	0
5	A	502	MPD	1	0
4	A	501	PC	1	0
5	A	504	MPD	1	0
5	B	1506	MPD	1	0
4	B	501	PC	1	0
5	A	503	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	305/308 (99%)	-0.08	10 (3%)	49	48	15, 24, 37, 51	1 (0%)
1	B	308/308 (100%)	-0.13	10 (3%)	50	49	15, 24, 38, 57	1 (0%)
All	All	613/616 (99%)	-0.10	20 (3%)	49	48	15, 24, 38, 57	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	SER	5.9
1	B	27	GLU	5.6
1	A	30	GLY	5.1
1	A	198	SER	4.6
1	B	334	SER	4.4
1	B	197	SER	4.0
1	A	51	ASN	3.9
1	A	197	SER	3.9
1	A	175	GLY	3.8
1	B	198	SER	3.7
1	A	199	GLY	3.4
1	B	199	GLY	3.1
1	B	333	PRO	3.0
1	B	175	GLY	2.7
1	B	83	TYR	2.6
1	A	333	PRO	2.4
1	A	174	GLN	2.4
1	A	334	SER	2.4
1	B	320	ASP	2.3
1	A	320	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	B	1506	8/8	0.33	0.31	61,62,63,65	0
5	MPD	A	505	8/8	0.52	0.27	54,56,60,60	0
5	MPD	B	1505	8/8	0.58	0.28	62,63,63,66	0
5	MPD	B	1502	8/8	0.63	0.25	61,63,64,65	0
5	MPD	A	504	8/8	0.65	0.21	55,56,56,57	0
5	MPD	B	1504	8/8	0.71	0.24	57,59,61,63	0
5	MPD	A	502	8/8	0.75	0.19	53,54,58,58	0
5	MPD	A	503	8/8	0.77	0.19	52,53,54,55	0
5	MPD	B	1503	8/8	0.78	0.18	53,56,59,59	0
5	MPD	A	506	8/8	0.81	0.18	52,52,52,53	8
5	MPD	A	507	8/8	0.83	0.18	52,52,53,53	8
4	PC	B	501	11/11	0.96	0.11	20,29,36,36	0
4	PC	A	501	11/11	0.96	0.10	18,27,32,34	0
3	CA	B	403	1/1	0.99	0.04	18,18,18,18	0
3	CA	B	404	1/1	0.99	0.04	21,21,21,21	0
3	CA	A	404	1/1	0.99	0.03	17,17,17,17	0
2	FE	A	402	1/1	1.00	0.02	19,19,19,19	0
2	FE	B	401	1/1	1.00	0.01	19,19,19,19	0
2	FE	B	402	1/1	1.00	0.01	19,19,19,19	0
3	CA	A	403	1/1	1.00	0.02	19,19,19,19	0
2	FE	A	401	1/1	1.00	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.